Thoughts on Surrogate Fuels for Combustion

Med Colket

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Surrogate Fuels

- Definition
- Purpose
- Selection
- Costs
- Test Sensitivities
- Experience

Definition

- Surrogate fuel – A mixture of a small set of individual hydrocarbon ‘species’ or components in a specific mixture ratio that when combined replicate the behavior of a real fuel

- Applications to GT (aero), IGT, Diesel, SI

Purpose

In the case of a surrogate for combustion….

- Primary: For Modeling
  - We cannot yet capture the combustion characteristics of a real fuel – except for simplified problems in CFD simulations. Lack of accurate kinetic description is likely a contributor to this problem
  - Capturing the fuel chemistry of a real fuel will remain unachievable for the foreseeable future
  - Establishing the chemistry os one step towards a new CFD capability
- Secondary: For Validation
  - Proof. There is no guarantee that a surrogate can successfully achieve this goal. Experimental validation is a logical follow-on step
- Tertiary: For Sensitivities
  - Once surrogate is established, sensitivities to changes in the physical or chemical nature of the fuel can be examined

Questions?

- Modeling –
  - Can a few components truly simulate real fuel behavior?
  - Can a reaction model be constructed that (accurately) simulates the individual components, the surrogate, let alone the real fuel?
  - Fuel interaction effects?
  - What accuracy level is required?
  - How to prove this can work?
  - how to establish accuracy requirements?
  - How to simplify for practical CFD?
- Validation –
  - Accuracy requirements for experiment?
  - Range of data? (P/T, f/a, spray)
  - Costs? – forces use of solvents and impose complications to kinetic models

Selection of Surrogates

- No unique solutions
- Targets:
  - Selection of components – limited by availability of kinetic models
  - Selection of targets –
    - Ideally to match combustion (entire) characteristics
    - Treatment of both physical and chemical dependencies
    - So far done by personal preference…..or limitations
- Few robust, well defined methods

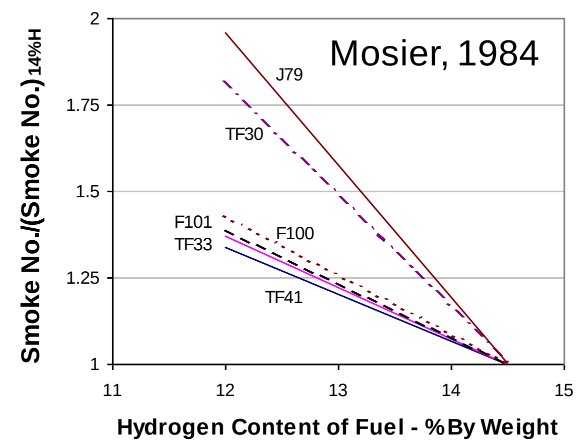
More Questions

- Can we ensure that matching a few selected targets guarantees matching all combustion characteristics?
- If not what are the limits in accuracy, or inability to match certain behavior?
- What specific targets are needed to match the ‘full set’; or a reduced set of combustion characteristics
- Is it acceptable to match a limited set of combustion characteristics? Does everything need to be matched?
- Are there specific characteristics that must be matched? – What are they?

Targets – proposed (for combustion)

- Chemical classes (n-alkanes, i-alkanes, cycloalkanes, aromatics…)
- Chemical groups (-CH2-, -CH3, -iC4H9, C7H7-, C6H11-, …..)
- TSI
- Ave MW
- CN, Ignition
- Boiling point (T10, T50, T90)
- H/C
- Premixed/Nonpremixed Extinction
- Liquid density
- Viscosity, surface tension
- ……
- Various combinations thereof
- Interdependency of properties?
- Mixing rules?????

Relationship between Smoke Number and Hydrogen Content



Relationship is not universal

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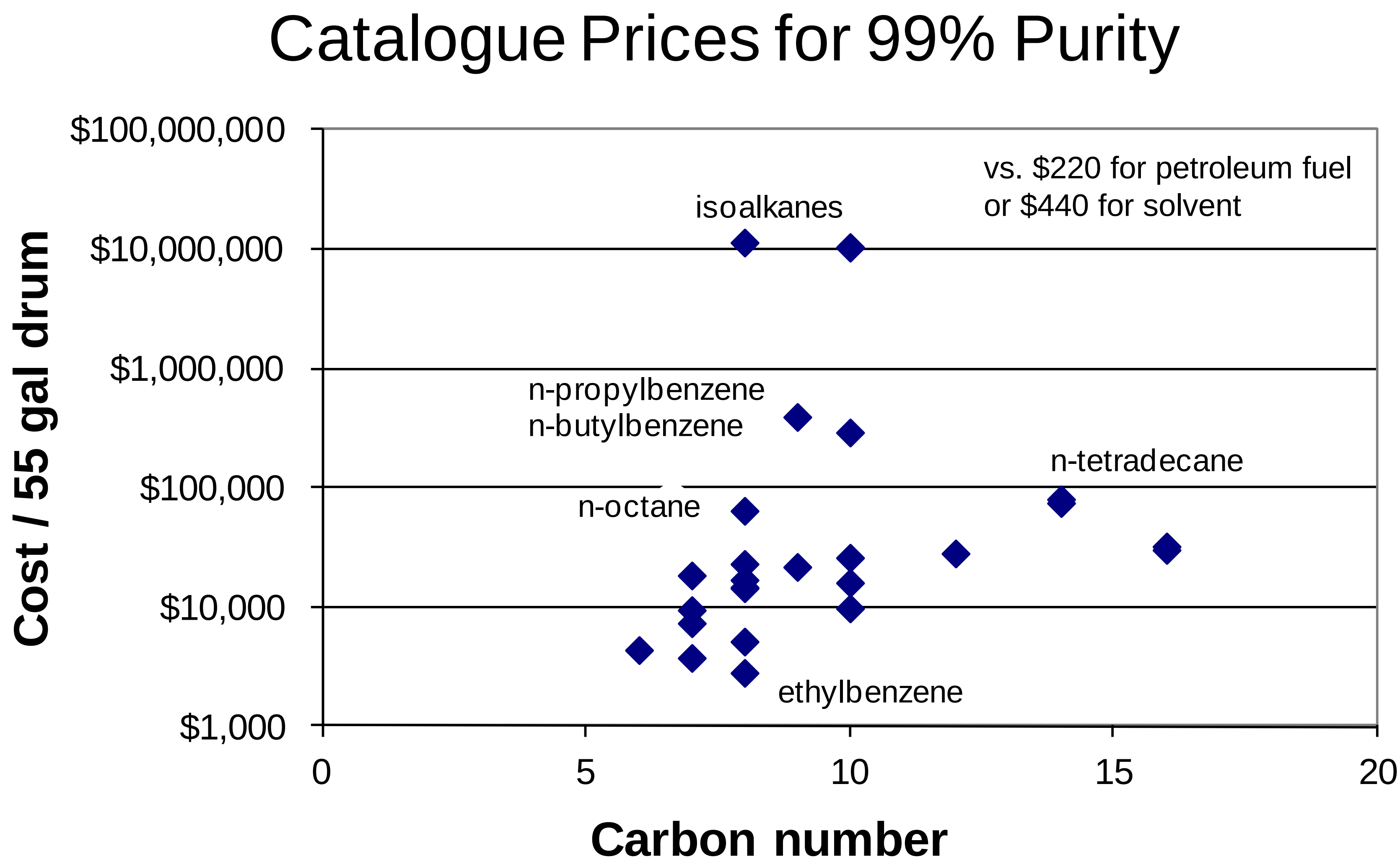
Relationship of targets to combustion characteristics?

Costs – Astronomical for High MW Pure Fuels



Solvents are the only real option for validation!

Sensitivities

Solvents/Surrogates can explore contrasting physical and chemical changes

		JP-5 (petroleum)	HRJ-5 (Camelina)	Sasol IPK	Shell GTL	Linpar 1416	L-142	L-210
JP-5 (petroleum)								
HRJ-5 (Camelina)								
Sasol IPK	Primarily iso-alkanes, some cyclo, C9-C14				Similar MW (C10), different chemistry (role of n-alkanes)		Similar MW (C10), different chemistry (iso vs. cyclo)	Similar chemistry, different MW (C10 vs. C14)
Shell GTL	isoalkanes and normal alkanes, C9-C12					Similar chemistry (not exact), different MW (C10 vs C14)	Similar MW (C10), different chemistry (Cyclo vs. norm)	
Linpar 1416	n-alkanes, C14-C16						Different chemistry, different MW	Similar MW (C14), different chemistry
L-142	Cycloalkanes, and some isoalkanes, C8-C13							Different MW (C10 vs C14) with simlar chemistry
L-210	Isoalkanes and some cycloalkanes, C13-C16							

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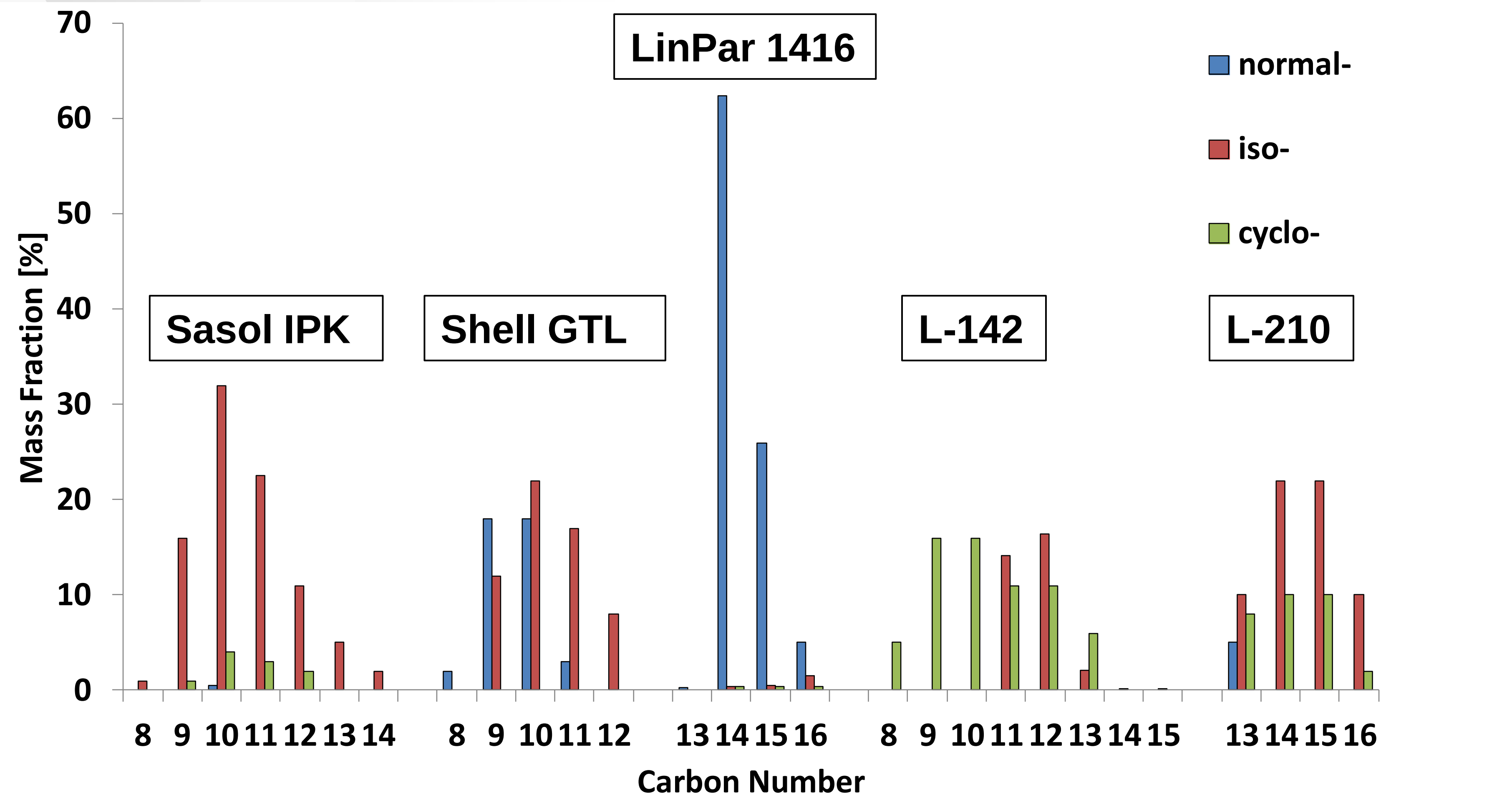
Experience

Encouraging results – but we have not closed the loop yet

- MURI
- Utah
- USC
- UTRC
- UC Irvine
- Europe
- UCSD

Combustor Validation Data – Fuels

Solvents and synthetic fuels explore contrasting physical/chemical changes



Wide range of chemical properties

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(cyclo: sum of monocyclic and dicyclic compounds